Study on Structure of GeTe Layer in GeTe/Sb_2Te_3 Superlattice Film

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ABSTRACT

The GeTe/Sb_2Te_3 superlattice (SL) film has been proposed for low-power phase-change memories according to Ge switching. The crystalline structure of the GeTe layer, which is one of the keys for low-power Ge switching, was studied by estimating the order parameter *S* using the XRD peaks of GeTe(111) and GeTe(222). The estimated *S* indicated that there are vacancies in the GeTe layer. Among the possible models for the vacancies, three models satisfied the allowable value $0.7 \leq S \leq 1.0$, one of which well agreed with the previously published result of the first principle calculation. In this paper, the possibilities of these models are discussed.

Key words: phase-change memory, superlattice phase-change film, interfacial phase-change memory

1. INTRODUCTION

A phase change random access memory is expected to be the next generation non-volatile solid-state memory[1]. Recently "interfacial phase change memory" with the superlattice (SL) structure has been proposed to suppress the switching power drastically[2]. In a GeTe(111)/Sb_2Te_3(001) SL film, Ge atoms reversibly switch between octahedral and tetrahedral sites depending on the applied voltages. This mechanism has been confirmed both experimentally[2] and theoretically using the first principle calculation[3]. In the calculation, the imaginary vacancy layer was incorporated in the GeTe layer. This vacancy layer is essential for Ge switching because the vacancy layer supplies the atoms the space to move relatively freely. The existence of this vacancy layer, however, has never been confirmed experimentally. In this study, the details of the SL structure were investigated using XRD data analysis.

2. EXPERIMENT

The procedure of the analysis is as follows. Firstly, all the possible configurations for GeTe crystalline structures with and without vacancies were modeled. The theoretical integral peak-intensity ratios $(I_{111}/I_{222})_{cal}$ were calculated for all the configurations. The experimental integral peak-intensity ratio $(I_{111}/I_{222})_{obs}$ was estimated using XRD data. The order parameter *S* is defined as

$$S^2 = \frac{(I_{111}/I_{222})_{obs}}{(I_{111}/I_{222})_{cal}}.$$

One of the configurations which satisfy $0.7 \leq S \leq 1.0$ should be the real configuration [4,5].

3. RESULTS AND DISCUSSIONS

XRD data of GeTe/Sb_2Te_3 SL film is shown in Fig.1. GeTe with no vacancy has $S \approx 1.76$. Thus, there must be vacancies in the GeTe layer. The above-mentioned analysis showed that three configurations shown in Fig. 2 satisfy $0.7 \leq S \leq 1.0$.

We cannot determine under the status quo which one of the above three configurations is likely. However, we will discuss on which one is the most likely. In the configuration A of Fig. 2, the space of the vacancies is too narrow for Ge atoms to move freely. So, the configuration A does not seem likely. If the configuration B is true, the Te layer is firstly constructed when GeTe is sputtered (Note that Te(000) is at the same time the Te layer of Sb_2Te_3). However, the chemical bond of Ge-Te is considered to be stronger than van der Waals Te-Te bond. This seems true because the melting temperature of GeTe is higher than that of pure Te. Thus, the Ge layer is considered to be constructed first on the Te layer of Sb_2Te_3. So, the configuration B does not seem likely. The configuration C, therefore, seems the most likely. This configuration is equivalent to the configuration adopted in the first principle calculation in reference 3.

4. CONCLUSION

The crystalline structure of GeTe layer in the GeTe/Sb_2Te_3 superlattice was investigated by estimating the order parameter S using XRD data analysis. The analysis showed that the vacancy layer in reference 3 seems the most likely among the configurations which satisfy the allowable value $0.7 \leq S \leq 1.0$.

ACKNOWLEGDEMENT

This research is granted by the Japan Society for the Promotion of Science (JSPS) through the "Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program)," initiated by the Council for Science and Technology Policy (CSTP).

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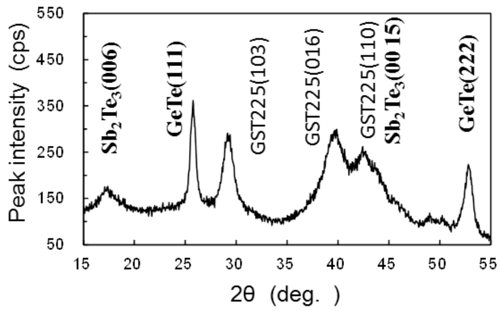

Figure 1 XRD data of GeTe/Sb_2Te_3 superlattice.

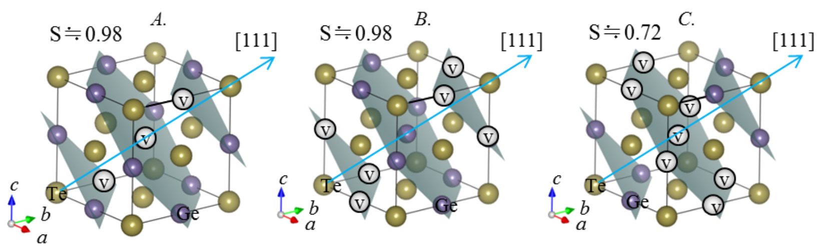

Figure 2 Vacancy layer configurations which satisfy $0.7 \leq S \leq 1.1$.